Influence of Thermal Fluctuations in Radiation Damage Cascade Production and Defect Dynamics in Tungsten

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1. INTRODUCTION

The detailed study of the deterioration suffered by the materials of the components of a nuclear facility, in particular those forming part of the reactor core, is a topic of great interest which importance derives in large technological and economic implications. Since changes in the atomic-structural properties of relevant components pose a risk to the smooth operation with clear consequences for security and life of the plant, controlling these factors is essential in any development of engineering design and implementation. In recent times, tungsten has been proposed as a structural material based on its good resistance to radiation, but still needs to be done an extensive study on the influence of temperature on the behavior of this material under radiation damage. This work aims to contribute in this regard. Molecular Dynamics (MD) simulations were carried out to determine the influence of temperature fluctuations on radiation damage production and evolution in Tungsten. We have particularly focused our study in the dynamics of defect creation, recombination, and diffusion properties. PKA energies were sampled in a range from 5 to 50 KeV. Three different temperature scenarios were analyzed, from very low temperatures (0-200K), up to high temperature conditions (300-500 K). We studied the creation of defects, vacancies and interstitials, recombination rates, diffusion properties, cluster formation, their size and evolution. Simulations were performed using Lammps and the Zhou EAM potential for W.

2. APPLICATIONS

Multiple applications have been proposed for tungsten, these include magnetic and inertial fusion reactors (iTER, HiPER and NIF) and fission reactors (VHTR)

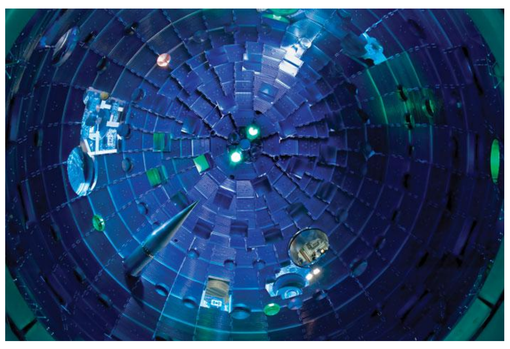


Figure 2.1: NIF Target Chamber

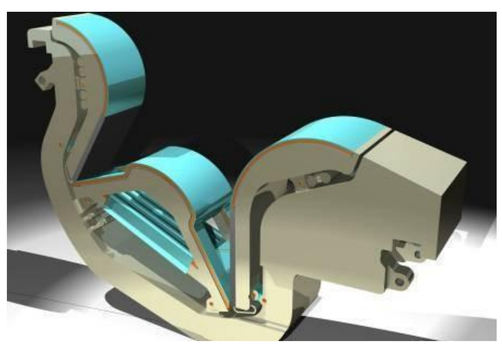


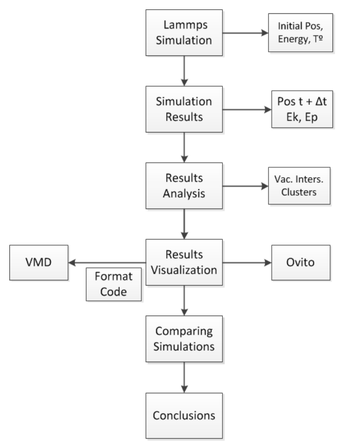
Figure 2.2: The three plasma-facing components of the ITER Divertor: the inner and the outer vertical targets, and the dome.

The detailed study of the deterioration suffered by the structural materials of a nuclear plant component, in particular those forming part of the reactor core, is a topic of great current work and importance derives in large technological and economic implications. Since changes in the atomic-structural properties of relevant components pose a risk to the smooth operation with clear consequences for security and life of the plant, controlling these factors is essential in any development of engineering design and implementation.

One of the consequences of the interaction of high energy particles (neutrons, ions or electrons) with crystalline materials is the formation of lattice defects resulting from the energy transfer towards the atoms. A very useful and widely used standard has been proposed by Norget, Torrens and Robinson in 1975 to evaluate the number of Frenkel pairs formed for a given energy transferred to the primary knocked on atom, and therefore the number of "displacements per atom", or so-called NRT-dpa (or just dpa in short). This evaluation of the primary damage suffers a number of limitations. First, it does not account for the recombination of atoms occurring during the cascade process. Molecular Dynamics simulations have shown for more than a decade that the number of defects remaining after the cascade is only about a third of the NRT rule. Second, this simple standard does not account for the nature and spatial distribution of the defects, which are also very important for the subsequent time evolution of the defect population. Third, the dpa value is inversely proportional to the displacement threshold energy; but this quantity is itself not very robust. The consequences of these limitations are that it becomes very difficult to compare the primary damage resulting from different irradiation conditions (nature of damaging particles and their energy spectra), or different materials.

3. METHODOLOGY

- Development of a code scheme for defect simulation and analysis.



- Modeling thermal fluctuations. Lattice Heating scheme:

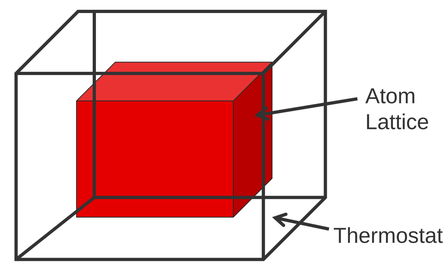


Figure 3.1: Scheme of atom lattice and thermal bath.

- Heat + equilibration: Berendsen and N-H Thermostats

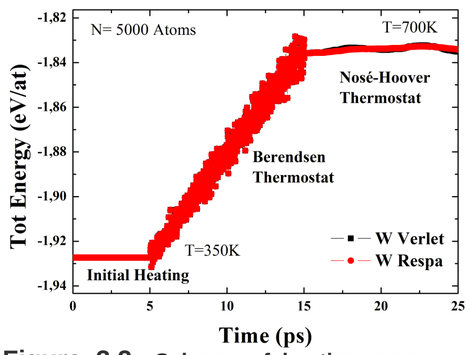


Figure 3.2: Scheme of heating process using Berendsen an N-H thermostats.

- Visualization (OVITO)

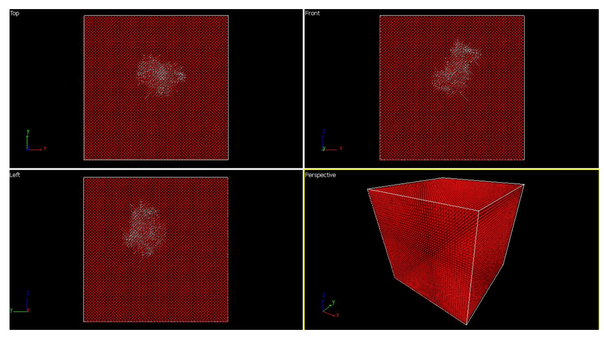


Figure 3.3: Displacement cascade in tungsten, displayed by Ovito.

4. Tungsten response to radiation damage. Comparison to other materials:

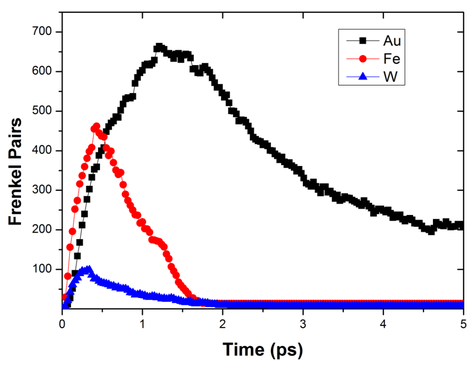


Figure 4.1: Evolution of Frenkel pairs identified for Au, Fe and W, with a 5 KeV PKA at 0 K for 5 ps.

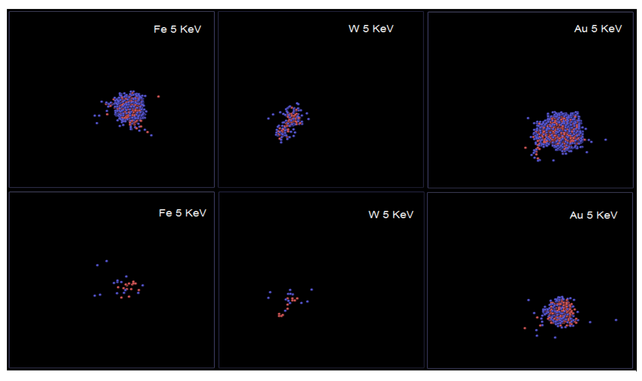


Figure 4.2: Comparison on displacement cascade at the maximum point of Frenkel pairs generation (top), and after finishing the stage of recombination (bottom) for Au, Fe and W , with a 5 KeV PKA at 0 K for 5ps MD time.

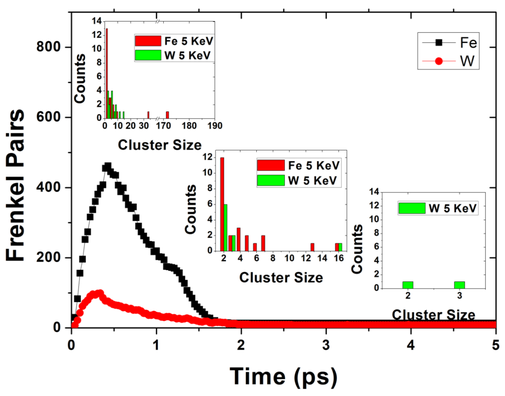


Figure 4.3: Comparison on cluster defects (vacancy clusters) evolution at different stages of the displacement cascaded for Fe and W, after a 5 KeV PKA at 0 K for 5ps MD.

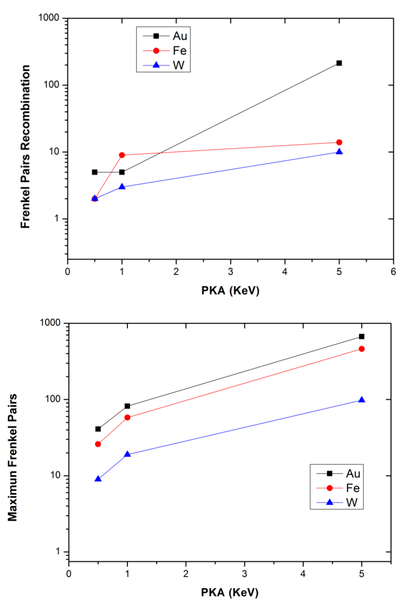


Figure 4.4: Maximum and resulting amount of Frenkel pairs after recombination for the studied compounds (Au, Fe and W) after three different PKA energy (0.5, 1 and 5 KeV). Results clearly show that tungsten is the material suffering from less Frenkel pairs, which is an expected result due to the higher hardness of this material. Furthermore, although the iron reaches a peak of defects much larger than tungsten these recombine reaching steady state in an amount slightly higher than the defects that survive in the tungsten. On the other hand, gold shows a generation of large quantities of defects, which is consistent with a material that is much softer than the iron and tungsten, and also shows a very poor recombination of Frenkel pairs. It is noteworthy that iron recombines in a better way and finally creates a similar amount of defects as W, however, it is expected that at bigger PKA energies (over 50 KeV) the difference between Fe and W will be enhanced.

5. Temperature Influence Over The Displacement Cascade & Evolution.

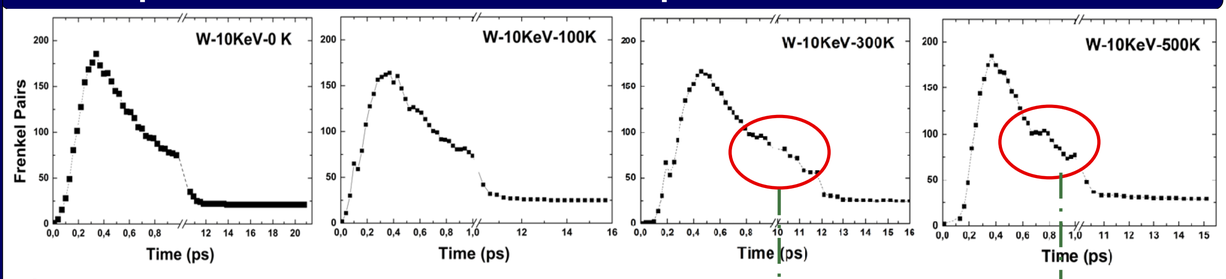
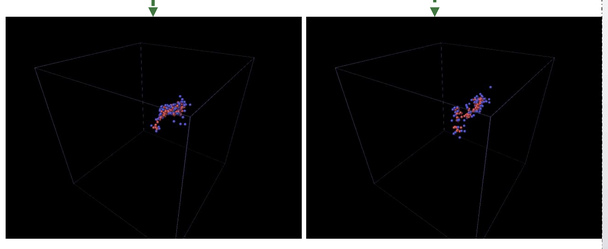


Figure 5.1: Evolution of Frenkel pairs identified for our four temperature scenarios: 0, 100, 300 and 500 K, for the last two cases we can observe the creation of ramification during the recombination stage, this affect and delay the recombination process.

Figure 5.2: 3D view of the displacement cascade for temperatures of 300 and 500 K, it seems that increasing the temperature produces a lengthening of the cascade that causes ramifications, they influence the shape of the cascade and how defects recombine and time recombination.



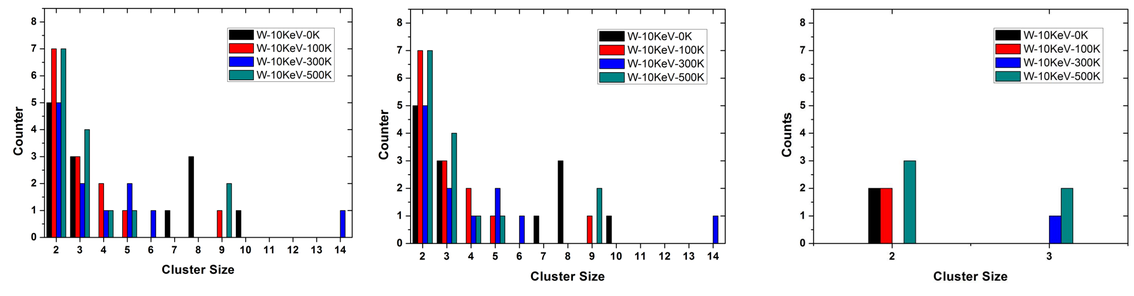


Figure 5.3: Size and number of clusters during the ballistic phase, recombination and once initiated the stabilization phase. The largest number of clusters occurs during the phase of maximum defect generation because there is a greater number of vacancies available to clump together. During the period of recombination, a diminution in cluster number and size is detected due to the disappearance of defects and large clusters no longer exist. Finally, in the stabilization phase we see that large clusters have completely disappeared and only a couple of size 2 or 3 vacancies survives, this confirms the hypothesis that the tungsten has a good resistance to irradiation.

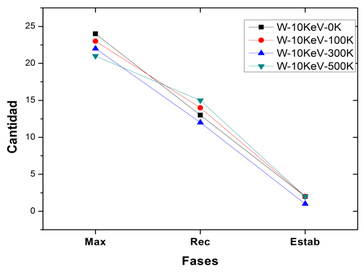


Figure 5.4: Total number of vacancy clusters generated in the three stages followed by our analysis, one can visualize how the total number decreases as the defects recombine and once reached the stabilization phase the final amount is almost the same for all cases studied. Thermal fluctuations clearly influence in both the generation and recombination phases.

6. CONCLUSIONS

- **Better resistance to radiation damage of tungsten versus other materials**
- **Good rate of recombination of tungsten (PKA > 50 KeV → Frenkel pairs W < Fe).**
- **There is an influence of temperature on recombination: Features and speed.**
- **There is an influence of temperature on the form typology that takes the displacement cascade: ↑ T → ∃ Ramifications.**
- **Ramifications affecting the way in which recombine defects → ↑ Recombination time.**

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